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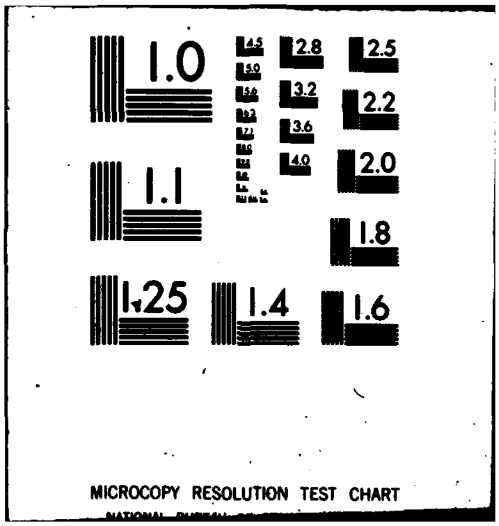
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FINDING THE GLOBAL MINIMUM OF A FUNCTION OF ONE VARIABLE USING THE METHOD OF CONSTANT SIGNED HIGHER ORDER DERIVATIVES

by

10 Garth P. McCormick

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by

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1. Introduction

The one variable minimization problem

$$\text{minimize} \quad f(x) \text{ s.t. } \; L \leq x \leq U \tag{1}$$

is important in optimization theory because it often arises as a subalgorithm for solving general constrained nonlinear programming problems in several variables. Convergence proofs for some standard methods (see e.g. [7], [8]) assume that either the first smallest local minimizer for the problem be found, or that a global minimizer is obtained. (A local minimizer is a point associated with a local minimum to the problem.) When $f(x)$ is not a unimodal function, standard algorithms for solving (1) may yield minimizers which are neither the first, nor the global ones.

In this paper a new method based on simple observations is presented for finding a global minimizer of (1). This method applies when the function to be minimized has continuous derivatives of higher order. It is further restricted to cases where the number of zeros of the derivative of $f(x)$ in $[L,U]$ is finite. It is not difficult to find functions (e.g., $x\sin(1/x)$, $0 \leq x \leq \pi/2$) which do not satisfy this restriction. For most practical

problems this presents no difficulty. The computational requirements, i.e., actually computing the higher order derivatives, are met for a large class of functions called Factorable Functions (see [2], [4]) using formulas developed in [6]. This aspect of the problem will not be further commented on here.

This new method is also an alternative to the method of Goldstein and Price [3] for finding the global minimizers of polynomials.

2. Preliminary Theorems and Lemmas

The algorithm for finding global minimizers is based on three simple theorems, all of which are well known. The first one states the obvious fact that finding all the zeros of the first derivative in an interval is equivalent to finding the global minimizer.

Theorem 1. Suppose $f:E^1 \to E^1$ is once continuously differentiable in the interval $[L,U]$. Suppose that there are p zeros of the derivative in that interval and that they are known and ordered as $L \leq z_1 < z_2 < \cdots < z_p \leq U$. Then a global minimizer for the problem $\min f(x)$ s.t. $x \in [L,U]$ must be one of $L, \{z_i\}$ $i=1,\ldots,p$, U.

Proof. A well-known necessary condition that a point in (L,U) be local unconstrained minimizer is that the point be a zero of the derivative. Thus if a global minimizer is an interior point, it must be one of $z_1,\ldots,z_p$. If it is a boundary point it obviously must be one of L or U.

The second theorem asserts that a function is strictly monotone in an interval if its derivative has constant sign there. Furthermore the function can have at most one zero there and a simple test determines whether it does.

Theorem 2. Suppose $f:E^1 \to E^1$ is kth continuously differentiable in the interval $[a,b]$. Suppose further that $f^k(x) > 0$ (<0) in (a,b). Then $f^{i-1}(x)$ is strictly monotone increasing (decreasing) in $[a,b]$, and there is only one possible zero of $f^{k-1}(x)$ in $[a,b]$. Specifically, if $f^{k-1}(a) \cdot f^{k-1}(b) \leq 0$, there is exactly one zero there, and if

$f^{k-1}(a) \cdot f^{k-1}(b) > 0$, there is no zero in that interval.

Proof. From the mean value theorem, for any $y,z \in [a,b]$,

$$f^{k-1}(y) - f^{k-1}(z) = f^k(n)(y-z) \quad \text{for some} \quad n \in (a,b) .$$

The monotonicity follows directly from this equality and the assumption that $f^k(x) > 0$ (< 0) in (a,b) .

If $f^{k-1}(a) \cdot f^{k-1}(b) \leq 0$, then one is greater than or equal to zero and the other is less than or equal to zero. Continuity of f^{k-1} implies the existence of at least one point where f^{k-1} is zero. The strict monotonicity shown above proves that only one such point exists in the interval.

If $f^{k-1}(a) \cdot f^{k-1}(b) > 0$, then both values have the same sign. The monotonicity property then implies all in between values are of that sign, Q.E.D.

The third theorem provides the basis for the upward process of the global minimizing algorithm. It says essentially that if all the zeros of a function's first derivative are known (in an interval), then the function itself can have at most one more zero. Furthermore the zeros of the first derivative (with the interval endpoints) provide the intervals in which the zeros of the function are located, (one possible zero in each interval).

Theorem 3. Suppose $f:E^1 \to E^1$ is kth continuously differentiable in the interval $[\hat{L},\hat{U}]$. Suppose that f^k has q zeros in that interval and that they are known and ordered as $\hat{L} \leq z_1 < z_2 \ldots < z_q \leq \hat{U}$. Then $f^{k-1}(x)$ is strictly monotone in $[\hat{L},z_1]$, $[z_i,z_{i+1}]$ (for $i=1,\ldots,q-1$), and $[z_q,\hat{U}]$. There are at most $q+1$ zeros of f^{k-1} in $[\hat{L},\hat{U}]$. Specifically, there may be one in $[\hat{L},z_1]$, one in each of $[z_i,z_{i+1}]$ (for $i=1,\ldots,q-1$) , and one in $[z_q,\hat{U}]$. If $f^{k-1}(\hat{L}) \cdot f^{k-1}(z_1) > 0$ there is no zero in that interval, otherwise, there is exactly one there. If (for $i=1,\ldots,q-1$) $f^{k-1}(z_i) \cdot f^{i-1}(z_{i+1}) > 0$,

there is no zero in that interval, otherwise there is exactly one. Finally, if $f^{k-1}(z_q)\cdot f^{k-1}(\hat{U}) > 0$ there is no zero in $[z_q,\hat{U}]$. Otherwise, there is exactly one.

Proof. Since $f^k(z_i) = f^k(z_{i+1}) = 0$, and there are no zeros between z_i and z_{i+1} , then $f^k(x) > 0$ for all $x \varepsilon (z_i,z_{i+1})$, or $f^k(x) < 0$ in that open interval. Thus the hypotheses of the previous theorem are satisfied and the appropriate conclusion follows for $[z_i,z_{i+1}]$. The other cases are identical.

The last theorem provides a rationale for eliminating subintervals from consideration as locations of the global minimizers if information concerning an approximation to the global minimum value is available.

Theorem 4. Suppose $f(x)$ is a continuous scalar function in the interval $[L,U]$. Let x_0 be a point in $[L,U]$ whose function value is known (i.e., $f(x_0)$ has been computed). Then

$$\min\ f(x) \text{ s.t. } x\varepsilon[L,U] = \min\ f(x) \text{ s.t. } x\varepsilon\{x \mid f(x) \leq f(x_0),\ x\varepsilon[L,U]\} .$$

Proof. The proof is omitted.

3. Algorithmic Considerations

Central to the development of an algorithm based on the theorems of the previous section is the availability of a subalgorithm which is guaranteed to find the zero of a strictly monotonic function in an interval.

Let $\alpha(x)$ be a scalar valued function which is continuous and strictly monotonic in the interval $[a,b]$. Assume that $\alpha(a)\cdot a(b) \leq 0$. Consider the problem:

$$\text{find } \bar{x} \text{, the unique point in } [a,b] \text{ such that } \alpha(\bar{x}) = 0 . \qquad (2)$$

A method for solving this problem is called a Guaranteed Zeroizing Algorithm (GZA) if it is guaranteed to generate the solution in a finite number of steps, or generate an infinite sequence converging to $\bar{x}$.

One simple-minded GZA for solving problem (2) is as follows.

If $\alpha(a) = 0$ or $\alpha(b) = 0$, quit. Otherwise, assume without loss of generality, that $\alpha(a) < 0$ and $\alpha(b) > 0$. Set $a_0 = a, b_0 = b$. In general, at iteration k assume that $\bar{x}$ is known to lie in (a_k, b_k) . (Certainly by assumption this is true for $k=0$.) Calculate $\alpha(m_k)$ where $m_k = (a_k+b_k)/2$. If $\alpha(m_k) = 0$, set $\bar{x} = m_k$ and quit. Otherwise, there are two possible cases.

If $\alpha(m_i) > 0$, set $a_{k+1} = a_k$, and $b_{k+1} = m_k$. Because of the assumption that $\alpha(x)$ is strictly monotonic increasing, $\bar{x}$ must lie in this interval.

If $\alpha(m_i) < 0$, set $a_{k+1} = m_k$, $b_{k+1} = b_k$. Again, $\bar{x}$ must lie in $[a_{k+1}, b_{k+1}]$. If the resulting interval is small enough, the algorithm is terminated. Otherwise the $(k+1)^{st}$ iteration is initiated.

There are many "faster" methods for attempting to solve (2). If the function $\alpha(x)$ is continuously differentiable in $[a,b]$, then Newton's method can apply. This takes the form

$$x_{k+1} = x_k - \alpha^1(x_k)^{-1}\alpha(x_k) .$$

The method of golden sections can be applied by minimizing (or maximizing depending upon whether $\alpha(x)$ is monotone increasing or monotone decreasing) the function

$$\int_a^x \alpha(t)dt$$

in $[a,b]$. The secant method for this problem takes the form

$$x_{k+1} = [x_k\ \alpha(x_{k-1}) - x_{k-1}\ \alpha(x_k)] \ / \ [\alpha(x_{k-1}) - \alpha(x_k)] .$$

The method of golden sections is a GZA for Problem (2). Both Newton's method and the secant method can be modified so as to become GZAs. Without modification they can generate points outside $[a,b]$, or otherwise fail to converge.

There are many algorithms based on the theorems of Section 2 which can be used to find all the zeros of $f^1(x)$ in $[L,U]$, or find a global minimizer

of $f(x)$ in $[L,U]$ when the number of zeros of f^1 is finite in that interval. The basic idea, is first to divide the interval $[L,U]$ into subintervals, finding for each subinterval some derivative of f which has constant sign. Then, using the backward process implied by Theorem 3, each subinterval is analyzed, finding all the zeros of successive lower level derivatives of f until all the zeros of $f^1(x)$ in that subinterval (if any) have been located. Finally, the zeros over all the subintervals are examined (along with the endpoints L and U), and the global minimizers obtained. The results of Theorem 4 can be used also to eliminate from consideration any subinterval in which the function value is higher or equal to the lowest function value at a feasible point.

Essential to the development of an algorithm using the results of Theorem 3 is the capability of generating tight upper and lower bounds on derivatives of $f(x)$. For a large class of functions, called Factorable Functions, this capability is available. For references see [2], [4], and [6]. All that is required is the availability of interval bounds on simple functions of a single variable (sin, log, etc.). Complicated compositions of these simple functions make up most functions of a single variable. Bounds on sums and products and transformations of interval bounds are obtained through simple arithmetic computations. This aspect of the algorithm will not be elaborated on here. In the example some of the techniques are used.

The rigorous statement of the tight-bounding capability is as follows. Let $\{[L_i,U_i]\}$ be a sequence of nested intervals contained in $[L,U]$ such that $U_i - L_i \to 0$. An algorithm generates tight bounds on the kth derivative of f if it is capable of generating a sequence $\{v_L^{k,i}, v_U^{k,i}\}$ where for every i,

$$v_L^{i,i} \leq [\min f^k(x) \text{ s.t. } x \in [L_i,U_i]] \leq [\max f^k(x) \text{ s.t. } x \in [L_i,U_i]] \leq v_U^{k,i}$$

and $v_U^{k,i} - v_L^{k,i} \to 0$ as $U_i - L_i \to 0$.

These ideas will be applied to the problem: minimize $x\sin(x) - \exp(-x)$ subject to $x \in [0,2\pi]$. The graph of this function is given in Figure 1. There

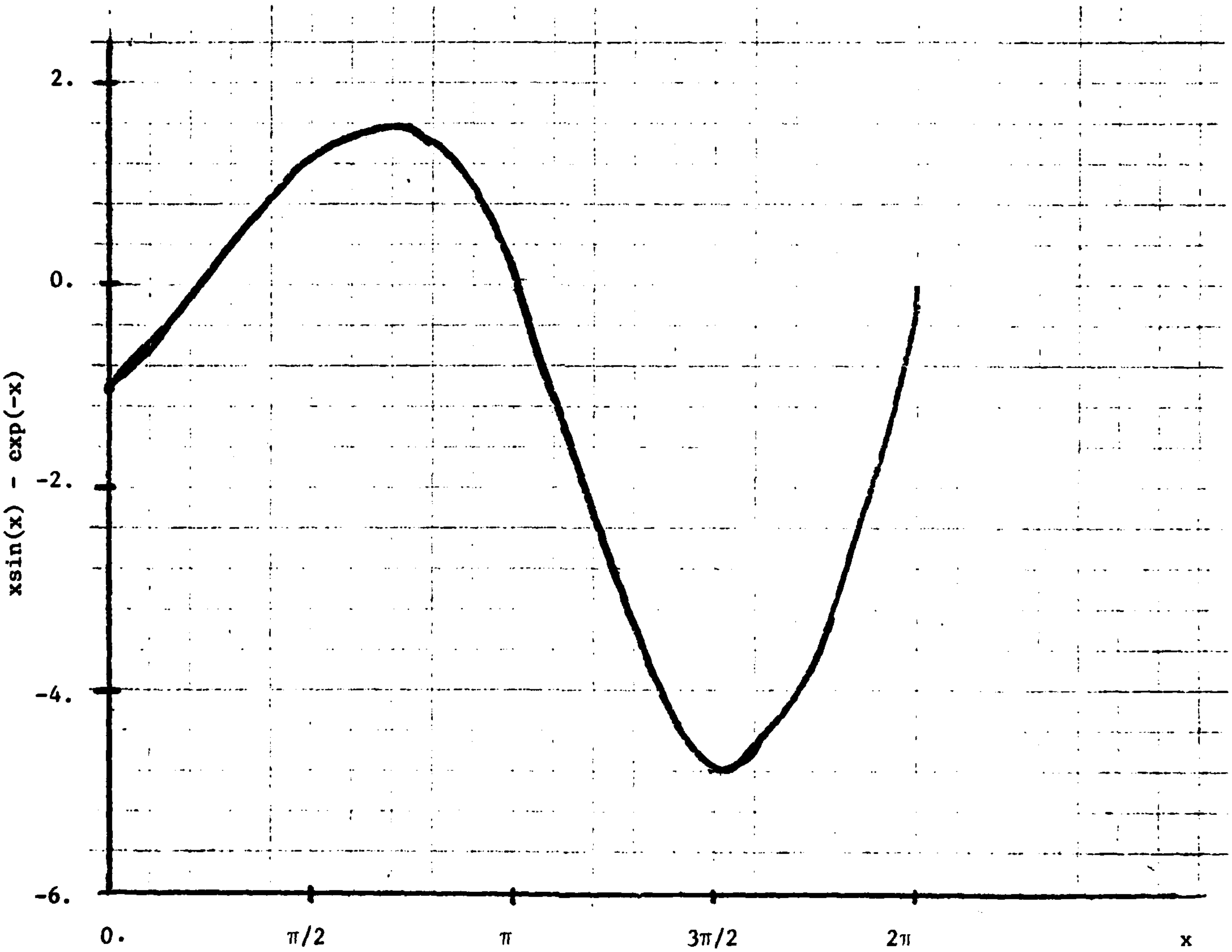

Figure 1. Graph of example problem.

are two local minimizers, one at 0., and the other at 4.911770 (= 1.563465 π). The successive derivatives take the forms:

$$f^1(x) = \sin(x) + x\cos(x) + \exp(-x) ,$$

$$f^2(x) = 2\cos(x) - x\sin(x) - \exp(-x) ,$$

$$f^3(x) = -3\sin(x) - x\cos(x) + \exp(-x) .$$

In computing tight upper and lower bounds on these expressions the only capability assumed will be that of obtaining the exact upper and lower bounds on the forms: sin(x), cos(x), exp(-x) for x in a given interval contained in [0.,2π]. From these values the standard techniques of interval arithmetic (see [5] for a fuller discussion of these) are used to bound the products and sums. The general formulas used here are as follows. Suppose for x in [L,U], $a \le \alpha(x) \le b$, and $c \le \beta(x) \le d$. Then $a + c \le \alpha(x) + \beta(x) \le b + d$, and $\min[ac,ad,bc,bd] \le \alpha(x) \cdot \beta(x) \le \max[ac,ad,bc,bd]$. (Subtraction is dealt with in the obvious way.)

The results of Theorem 4 can be used if some preliminary one dimensional search routine is assumed to have been applied to the problem. Depending upon the parameters used by the routine it would have found either the local minimizer at 0., or that at 4.911770. It is assumed that the former is available, i.e., $x_0 = 0.$, and $f(x_0) = -1$.

The initial bounds on the first derivative in [0.,2π] are

$$-7.2813 \le f^1(x) \le 8.2832 .$$

This interval is divided into two halves, [0.,π] and [π,2π]. For $x \in [0.,\pi]$, $f(x) \ge -1$. Search in this interval is terminated since no better point than $x_0 = 0.$, $f(x_0) = -1$ can be found there. For $x \in [\pi,2\pi]$, $-6.3264 \le f(x) \le -.0019$, $-7.2813 \le f^1(x) \le 3.1848$, $-9.2832 \le f^2(x) \le 8.2813$. None of the three functions allow upward processing of this interval so it will be further subdivided into [π,3π/2] and [3π/2,2π]. For $x \in [\pi,3\pi/2]$,

$$-4,7556 \leq f(x) \leq -.0090$$

$$-5.7034 \leq f^1(x) \leq .0432$$

$$-2.0432 \leq f^2(x) \leq 4.7034$$

$$.0090 \leq f^3(x) \leq 7.7143 \ .$$

The lowest derivative with constant sign in that interval is the third. Thus the upward processing of this interval can begin once the remaining interval is examined and a derivative with constant sign found there.

For $x \varepsilon [3\pi/2, 2\pi]$, the first three derivatives have bounds containing zero. The interval is further subdivided into $[3\pi/2, 7\pi/4]$ and $[7\pi/4, 2\pi]$.

For $x \varepsilon [3\pi/2, 7\pi/4]$, the lowest derivative with constant sign is f^2 with $3.3232 \leq f^2(x) \leq 6.9079$. For $x \varepsilon [7\pi/4, 2\pi]$, the first derivative is positive with $3.1823 \leq f^1(x) \leq 6.2873$. Conceptually the situation is depicted in Figure 2.

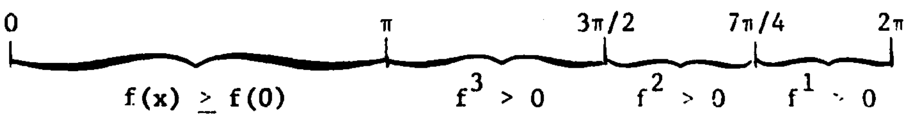

Figure 2. Derivative bounding information.

The upward processing of the intervals to find all the zeros of $f^1(x)$ now proceeds.

The interval $[\pi, 3\pi/2]$ is processed first. Here $f^3(x) > 0$. Now $f^2(\pi) = -2.0432$, $f^2(3\pi/2) = 4.7034$. Thus there is exactly one zero of f^2 in that interval. The secant method is used to find it. The successive iterations are given in Table 1.

Table 1

SECANT METHOD ITERATES

i	x_i	$f^2(x_i)$
0	π	-2.0432
1	$3\pi/2$	4.7034
2	3.6173	$-.1482$
3	3.6545	$.2477 \times 10^{-1}$
4	3.649236	$.168 \times 10^{-2}$
5	3.649199	$-.5189 \times 10^{-5}$

The point 3.649199 is the zero in that interval. The first derivative can have at most one zero in $[\pi, 3.649199]$ and at most one in $[3.649199, 3\pi/2]$ since the second derivative is monotone in each interval. Evaluating, $f^1(\pi) = -3.0983$, $f^1(3.649199) = -3.6491$, $f^1(3\pi/2) = -.9910$. Hence there is no zero to the derivative in either interval.

The second derivative is strictly positive in $[3\pi/2, 7\pi/4]$. Evaluating, $f^1(3\pi/2) = -.9910$, $f^1(7\pi/4) = 3.1845$. So there is exactly one zero there. Applying any GZA would yield the point 4.911770.

Since in the final interval $f^1 > 0$, obviously there are no zeros of the derivative there.

The process has been completed and the zero 4.911770 has been identified as the global minimizer for the problem. Note that if the interval $[0,\pi]$ had not been eliminated the above process would have found the local maximizer since the associated zero would have been located.

4. Application to Polynomial Minimization

The problem of finding the global minimizers of a polynomial relates to Problem (1) in the following way.

Consider the polynomial approximation to $f(x)$ using some point x_0 in $[L,U]$:

$$f(x) \doteq P^0(x) = f(x_0) + \sum_{i=1}^{k} f^i(x_0)(x-x_0)^i/i! \ .$$

The most that $f(x)$ and $P^0(x)$ can differ by is $\pm \varepsilon$, where

$$\varepsilon = [\max(|f^{k+1}_{min}|,|f^{k+1}_{max}|)] \ [\max(|U-x_0|,|L-x_0|)]^{k+1}/(k+1)! \ ,$$

where $f^{k+1}_{min} = \min f^{kH}(x)$ s.t. $L \le x \le U$, and

$$f^{k+1}_{max} = \max f^{k+1}(x) \text{ s.t. } L \le x \le U \ .$$

One approach for minimizing $f(x)$ in $[L,U]$ is to approximate it by a polynomial as above and minimize the polynomial. Depending upon the level of differentiability and the capability of computing the higher derivatives, the minimum of the polynomial can be made very close to that of the original function.

Using the results of Theorem 3 it is very simple to minimize the polynomial. The kth derivative is of constant sign (if it is zero the first nonvanishing derivative below the kth is used to start the process) and the process of finding the zeros of the successive polynomials

$P^k(x)$, $P^{k-1}(x), \ldots, P^1(x)$ can be initiated. This process is guaranteed to find all the zeros of $P^1(x)$ from which, by virtue of Theorem 1, all the local minimizers (and therefore the global minimizers of $P^0(x)$) can be determined.

The maximum amount of work now done in the upward process is the use of a GZA as many times as required. The most work is if each level contains one more zero finding problem. The work in this case would be $1+2+\ldots+(k-1) = k(k-1)/2$ zero finding problems. Hopefully, in practical problems the actual work would be less, and certainly at the highest level one would not expect more than three zeros of the derivative.

This algorithm is an alternative to that of Goldstein and Price [3] which "divides out" local minimizers from polynomials and eventually calculates all local minimizers of a polynomial. In Fiacco and McCormick [1] a worse case analysis shown that for a polynomial of degree k (k assumed even) the number of one dimensional minimization problems (yielding a local solution) could be as much as

$$k/2 + \sum_{i=1}^{(k/2-1)} [(k/2-i) \prod_{j=1}^{i} (k/2-j)] \ .$$

In addition, the Goldstein-Price scheme is subject to severe numerical problems since exact minimization is necessary in order to divide a polynomial of degree two into a higher degree polynomial to perform the analysis. This present scheme is relatively insensitive to numerical problems since the numbers obtained are endpoints of intervals.

5. Comment

For strictly convex programming problems the second derivative of the function $f(x)$ is greater than zero which implies the existence of at most one zero to the derivative. In step-size problems resulting from the minimization of a general convex function in several variables subject to points being restricted to a convex set, the step-size function is usually strictly convex. For nonconvex problems, the existence of more than one zero to a step size problem is rarely encountered. It does happen, and in such a circumstance the techniques

of these in this paper are applicable. In most cases just using first and second derivatives in a technique which divides the original into subintervals should suffice to obtain a global minimizer of a function in an interval.

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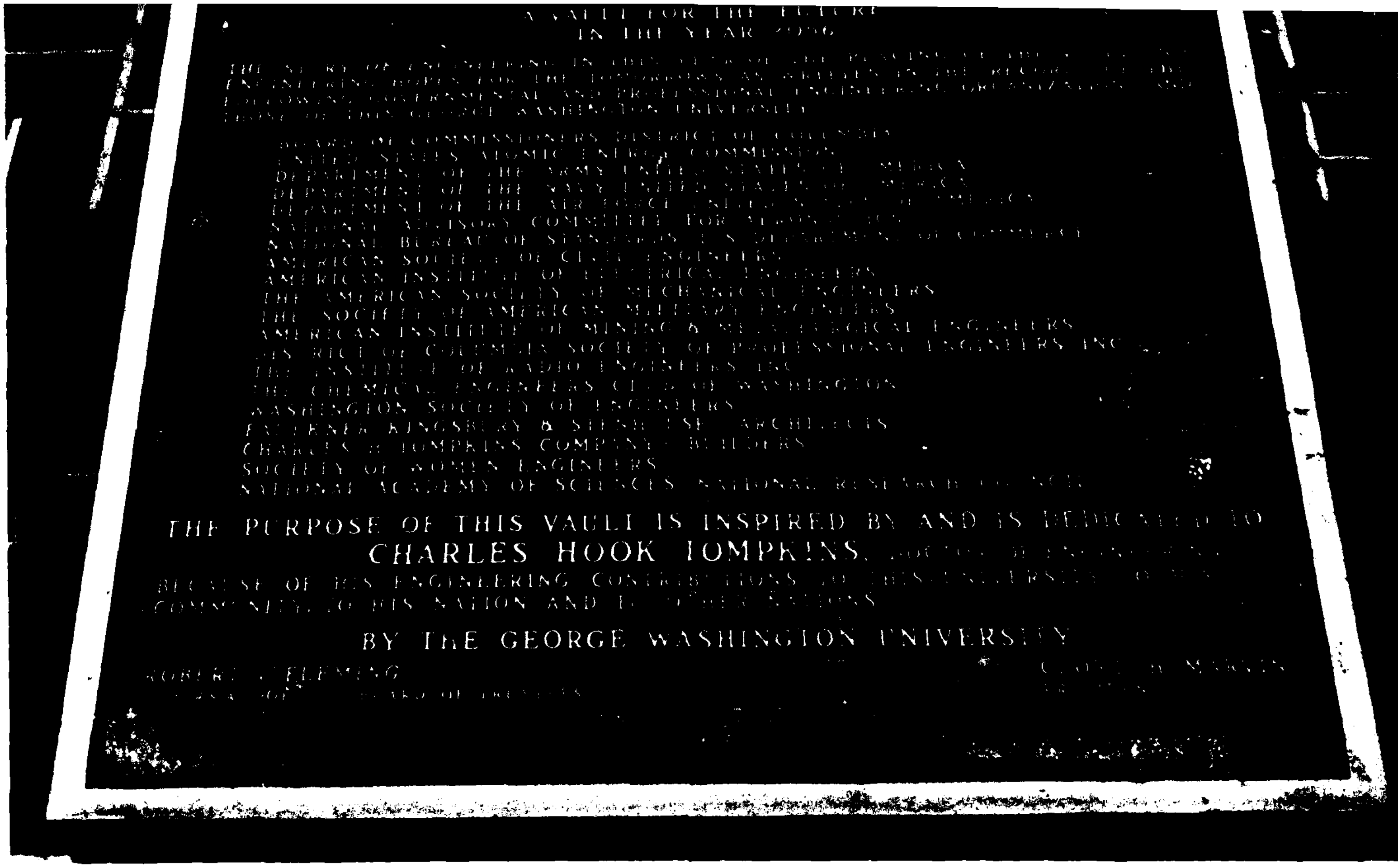

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